

Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt  
946-30-5 | DTXSID4061339

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

## Model Results

**Predicted value:** 312 °C

**Global applicability domain:** Outside

**Local applicability domain index:** 1.82e-01

**Confidence level:** 5.06e-01

## Nearest Neighbors from the Training Set

Image not found

Trimellitic anhydride

**Measured:** 390

**Predicted:** 366

Image not found

Chloramben

**Measured:** 312

**Predicted:** 301

Image not found

Benzoic acid, 2,4,5-trimethoxy-

**Measured:** 300

**Predicted:** 302

Image not found

Benzoic acid, 2-benzoyl-

**Measured:** 261

**Predicted:** 309